A Low Temperature Diffraction Study of La_{2-x}M_xCuO₄ and Related Compounds

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Introduction: The low temperature crystallographic transformation in La_{2-x}M_xCuO₄ (M=Ba or M=Nd,Sr) from the orthorhombic LTO1 phase (Bmab) to the low temperature tetragonal LTT phase (I4/mmm) is of great interest because of the associated effects on superconducting properties, and on charge stripe pinning. This high resolution powder x-ray diffraction study closely examines this transformation in light of low temperature transmission electron microscopy (TEM) work. In those samples, which transform to LTT, the powder diffraction and TEM both suggest a two step transformation. As temperature is reduced, a minority LTT phase appears in the LTO1 material, maintaining ~10% of the sample volume over a >50K range of temperature. At some lower temperature, typically near 60K, the sample transforms essentially completely to LTT over a range of ~10K. For samples which do not transform to LTT, (M=Sr and M=Ba for x<0.09), the partial transformation from LTO1 to LTT is still observed. Most recently this work has centered on the partial transformation to LTT in oxygen isotope-exchanged samples Sr~0.12. The variation in superconducting transition temperature T_c with oxygen isotope exchange and with composition Sr x has long attracted attention (Crawford). In this work we re-examine the low temperature structures of oxygen isotope exchanged powder specimens. The usual source for isotope effects in superconductors is the interaction of the electronic structure with the perturbed phonon spectrum. The objective here is to eliminate the possibility that subtle physical structural differences contribute to these samples properties.

Methods and Materials: The polycrystalline samples (M=Sr, x~0.1125) are those reported on in a previous study of isotope exchanged samples. Powdered samples were mounted on a flat copper plate, then put into a continuously operating helium refrigerator capable of attaining a temperature T=20K. X-ray diffraction data was obtained at NSLS X7A, configured with a crystal analyzer, using ~0.7 nm wavelength. The LTO1 020/200 peak region was carefully monitored for presence of minority LTT phase as well as LTO1 orthorhombic splitting. An example of two and three peak fits from an earlier study is shown in **Figure 1** (Moodenbaugh).

Results: Results for the isotope exchanged samples are shown in **Figure 2**. We conclude that, within the accuracy of the experimental x-ray diffraction data and the corresponding fits, the samples are indistinguishable.

Conclusions: It appears that the effect on superconductivity of oxygen isotope exchange in these materials cannot be attributed to crystallographic differences between the isotope exchanged samples.

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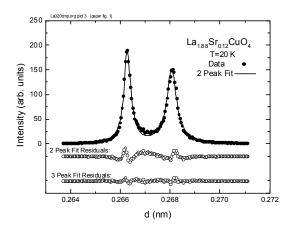


Figure 1. Peak fits illustrating the presence of two phases, a majority LTO1 phase and a minority LTT phase. The peak fitting is accurate when a broad LTT 200 peak is added to the LTO1 two peak, 020/200, fit.

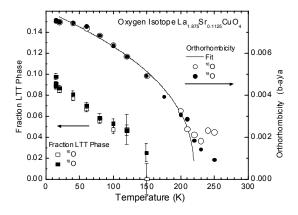


Figure 2. Analysis of the LTO1 020/200 peak region for isotope exchanges samples yields two parameters plotted as a function of temperature. The fraction of LTT phase is obtained from a three peak fit to the data, taking total intensity as a measure of phase fraction. The orthorhombicity is obtained from the fitted orthorhombic 020/200 peak positions.